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COMPLEX ROUTE TO CHAOS IN VELOCITY DRIVEN ATOMS*

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Complex route to chaos in velocity-driven atoms*

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Abstract

The oscillations of a linear triatomic molecule with the first atom driven at a constant velocity v are studied numerically. As v increases, we observe a sequence of transitions from quasiperiodicity to chaos, mode locking, chaos, another mode locking then to chaos before the atoms break off. The largest Lyapunov exponent does not rise linearly with the driven velocity. The mode locking structure for the last onset to chaos has a universal fractal dimension 0.871 ± 0.001 at a winding number far from the golden mean.

Many dissipative systems are known to undergo transitions to chaos by different routes. Such transitions in a system with few degrees of freedom may provide some insight into turbulence. The quasiperiodic transition has been observed experimentally[1,2] in the Rayleigh-Bénard convective fluid, thermo-acoustic oscillation, electronic conduction in extrinsic Ge, Josephson junctions, charge density waves, and many others. These are some of the experiments that could be modeled by the circle map. Recent theoretical developments have resulted in some quantitative and universal characterizations for the onset of chaos[3]. In most of experiments on the quasiperiodic transition, one of the two frequencies can be varied directly. This allows the ratio of the two frequencies (or winding number) to be set arbitrarily close to a value corresponding to the golden mean ($0.61803...$) where one can expect to observe a universal scaling behavior at the onset of chaos as predicted by theory. In some experiments, however, the two frequencies arise intrinsically from the system and can not be controlled directly. In these cases, for example the Rayleigh-Bénard convective ^{4}He fluid[4], it is somewhat difficult to achieve the golden mean ratio. However, the system exhibits a quasiperiodic transition to chaos with a mode locking staircase that has a fractal dimension D close to 0.868 in good agreement with theoretical predictions by the circle map. As predicted, this universal value of D is a global property and should hold not only at the golden mean but also for a range of winding number at the onset of chaos[3,5]. Futhermore, many condensed matter systems are known to undergo transitions to chaos when there is a competition between two incommensurate frequencies which is not necessarily at the golden mean.

In our model, we observed a different route to chaos beginning with two incommensurate frequencies. The external control parameter can only vary both frequencies indirectly. After the first transition to chaos, there is an abrupt transition to mode locking that gives rise to the first section of an incomplete devil's staircase amidst a set of quasiperiodic points. This is followed by a window of chaos then another section of a mode-locked staircase, then comes the last stage of chaos before the disappearance of the attractor signaling a separation of the atoms.

The atomic motions in a gas or fluid driven by a high pressure front are likely to become turbulent. Molecular dynamics studies of shock front propagation in solids often involve the so called   piston problem. In the one-dimensional version of this problem, one atom at the end of a long chain is driven at a constant velocity and the dynamics of the remaining atoms in the system is studied. The problem attracting our interest is a simpler but related one. It consists of three identical atoms moving in a straight line with the first atom driven at a constant velocity v . These atoms are assumed to interact through a potential[6]

$$V_{i,j} = C[1 - K(x_i - x_j)]e^{-K(x_i - x_j)} \quad , \qquad (1)$$

where x_i is the position of the ith atom, K and C are positive constants proportional to the equilibrium separation and the binding energy respectively. As in the model containing many more atoms, this is a non-conservative system because a varied force is required to maintain a constant velocity of the first atom. Here we will investigate in detail the relative motions of the three atoms, focussing on the behavior of the bond length in response to different values of v. An immediate question concerns the value of v that causes the three atoms to break apart, and the chaotic behavior that may occur in the system.

We begin by integrating the following equations of motion

$$\frac{d^2Y_i}{dT^2} = (Y_{i+1} - Y_i - 2)e^{-(Y_{i+1} - Y_i)} - (Y_i - Y_{i-1} - 2)e^{-(Y_i - Y_{i-1})} \quad , \qquad (2)$$

where $Y_i = Kx_i$ and $T = \omega t$ are the new atomic position and time in dimensionless units respectively. The dimensions used in this calculation can be scaled so that each unit of velocity, distance and time correspond to 8.295 Km/sec, 0.55 Å and $\omega^{-1} = 6.63 \times 10^{-15}$ sec respectively. These values were based on an Nitrogen atomic mass of 14 amu, a bond length of 1.1 Å and binding energy of 5 eV. Any other type of atom will simply result in a different set of scaled units. We will consider the oscillations of the two bond lengths $B_1 = Y_2 - Y_1$ and $B_2 = Y_3 - Y_2$. In solving the set of ordinary differential equations, one may not wish to use the relative coordinates due to a constraint on the velocity of the first atom.

3

For an extremely small value of v, the atoms are near their equilibrium positions and their interaction can be approximated by a harmonic potential. Then the ratio of two natural frequencies of the system is known as $1/\sqrt{3}$. The two bonds start oscillating with two incommensurate frequencies. We will limit our discussion to the first bond near the shock front. As we increase v, harmonic frequencies of the form $mf_1 + nf_2$ begin to appear as seen in the power spectrum in Fig.1a. The phase space diagram shows a quasiperiodic attractor for the bond which oscillates about its equilibrium value of 2.0 (Fig.2a). The Poincaré section of this attractor is shown in Fig.3a. The first transition to chaos occurs when v reaches 0.267. The power spectrum develops broad band signals (Fig.1b), corrugations of the Poincaré section appear (Fig.3b) and trajectories in the phase space start wandering (Fig.2b). Fully developped chaos takes place when v reaches 0.29 with characteristics shown in Fig.1c, 2c and 3c.

A sudden transition to quasiperiodicity takes places when v reaches 0.3093. Then a mode locking begins at $v = 0.3098$ and continues until $v = 0.31281$. The corresponding winding numbers are 7/18 and 5/13 respectively. We found two other mode-locked ratios within this interval using the Farey tree sequence. The prospect of locating other mode-locked ratios within this interval is certain, but very time consuming. Interspersed among the mode-locked ratios are quasiperiodic points (Fig.4).

The second transition to chaos takes place when v is slightly greater than 0.31281. Similar chaotic behaviors in the phase space, Poincaré map and power spectrum are obtained. A second series of mode-locked states emerges when $0.31309 < v < 0.31700$. In this interval we also show four mode-locked ratios using the Farey tree. Of course, there are other mode-locked states and quasiperiodic states as before. For each mode-locked ratio, The Poincaré maps and phase space diagrams clearly show the number of resonances of trajectories corresponding to the numerators of the mode-locked ratios (Fig.5). The existence of quasiperiodic points among the plateaux in the two mode-locked intervals suggests that the devil's staircase is incomplete and the transition to chaos is far from criticality.

4

The third transition to chaos takes place as v is increased past 0.317. The chaotic states persist until $v = 0.36804$. By increasing v from below to above this value, the chaotic attractor severely deforms. Its amplitude of oscillation bursts into a linear motion as a result of a separation of the first two atoms. In another words the attractor disappears. The bond stops oscillating about its equilibrium position and keeps stretching out as time progresses.

Since the two portions of the mode-locked staircase are separated by an interval of chaos in which the fractal characteristic is discontinued, we compute the fractal dimension of each of the two sections of the staircase separately using the expression $\sum_{i=1}^{n}(s_i/s_t)^D = 1$, where s_i is the gap between two plateaux and s_t is the largest gap. We obtained $D = 0.915 \pm 0.001$ for the first section and $D = 0.871 \pm 0.001$ for the second one. The value of D for the second portion of the staircase is in good agreement with the universal value $D = 0.868 \pm 0.002$. The larger value of D for the first section may arise from a transition far from criticality, as this same value of D has been found in the scaling behavior for the charge density wave and Josephson junction[2]. It appears that the nonlinearity in this model is not a monotonic function of the control parameter v. Then it is not feasible to show whether the system is approaching chaos from below or above criticality, although D is less than unity.

The sequence of transitions is summarized in Fig.6 with three chaotic regimes CH1 to CH3 alternating among a quasiperiodic QP2 regime and two mode-locked staircases PL1 and PL2. The region to the right of CH3 marks a disappearance of the attractor, as the atoms become separated. We calculate the largest Lyapunov exponent λ for the attractors within each of the three chaotic intervals using the method based on the evolution of trajectories[7]. As shown in Fig.7, there is a nonlinear relation between the control parameter v and the level of chaos. After some fluctuations during the first chaotic interval, λ decreases in the second and last interval while remaining positive. In this model, the nonlinearity parameter is fixed (K), the factor that leads to a transition to chaos is due to the interaction of the external driven force, parameterized by the

velocity v, with a nonlinear potential. Significant nonlinearity will arise when the driven force with a large value of v interacts with higher order terms of K from the exponent in the potential. Driven nonlinear systems often generate both subharmonics and higher harmonics. In the first transition to chaos, higher harmonics ($mf_1 + nf_2$) were gradually suppressed. The lower fundamental frequency f_1 was the most stable component to dissappear at the onset of chaos. We do not know the exact mechanism for the repeated transition to chaos or for the reappearance of higher harmonics when the system goes from chaos to mode-locking. However, the indirect cause may be linked to the oscillation of the nonlinearity generated under different values of the driven velocity. This is reflected in the cu ve for the Lyapunov exponent.

There are systems in which chaos emerges regularly in parameter space. A well known example is the Belousov-Zhabotinsky reaction. This experiment[8] reveals that alternating regimes of chaos and periodicity appear regularly in a sequence of multiple bifurcations. In this case, the transition to chaos may be characterized by a different universal number but does not possess a mode locking structure and a fractal dimension as in our model. It is also known that experiments on the transition to chaos via mode locking exists[2,9] but the recurrence of chaos was not found in these models. In a particular Rayleigh-Bénard experiment[10] for a specific type of convective cells, it has been observed that the system transitioned from quasiperiodicity to chaos then to mode-locking at one winding number only, but no mode-locked structure has been found. We know of no previous results from experiments or theoretical models that exhibit a similar sequence of transitions to chaos like our model. We have also looked into a similar model with a much larger size, up to five hundred atoms in a linear chain. Similar attractors were found on groups of three atoms when the chain was driven by a strong front and broken into segments. However, the dynamics is very complex and the work is still underway. For a system with few degrees of freedom, this is the first model that exhibits recurrent transitions to chaos and a mode-locked staircase with a universal fractal dimension. It also provides some new details to the dynamical process of atoms interacting with a steady moving front.

Acknowledgement:

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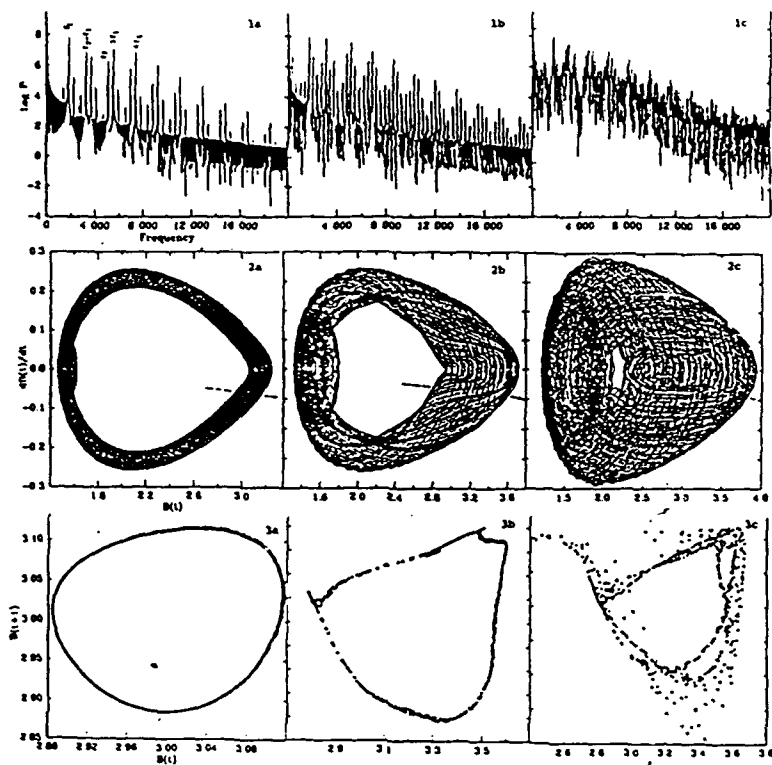[10] P. Bergé, Y. Pomeau and C. Vidal, *Order within chaos*, J. Wiley and Hermann (Paris), p.180 (1984).
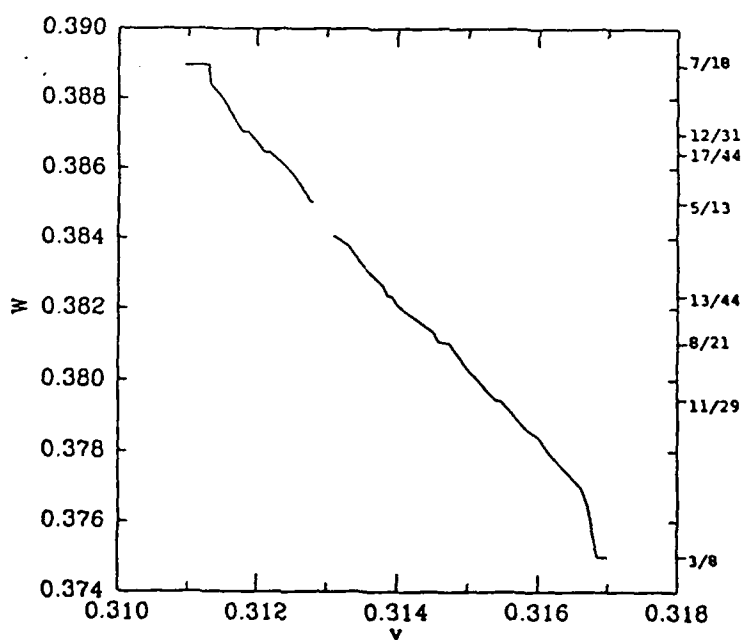
List of Figures:

Fig.1-3

Fig.4

Fig.5

Fig.6

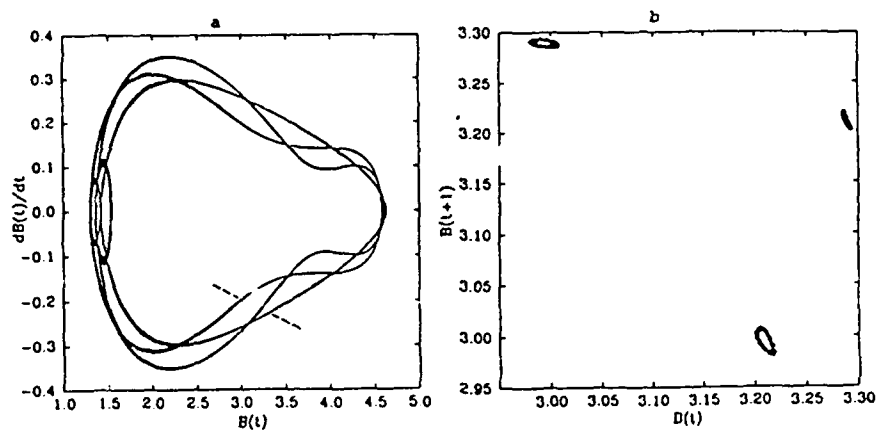
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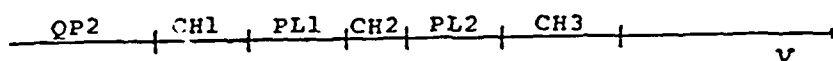
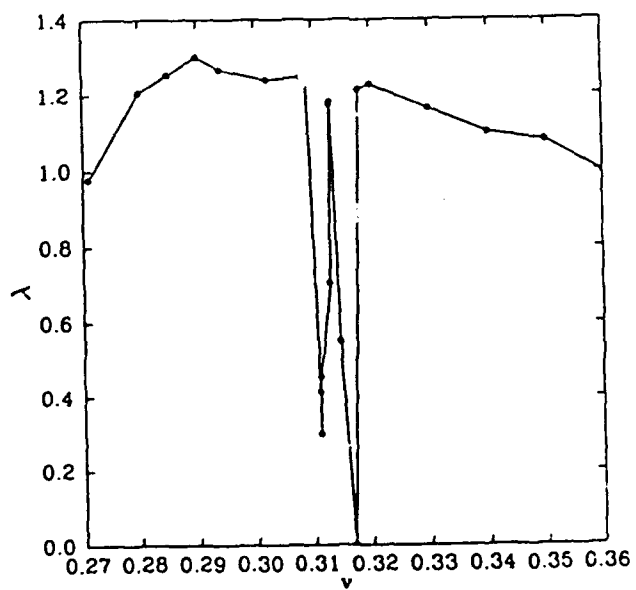REPORTS DISTRIBUTION FOR ONR PHYSICS DIVISION
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Page 3 of Enclosure (2)